§13. Research on Formation of Dust in Fusion Device Using Infrared Spectroscopy

Kenmotsu, T., Wada, M. (Doshisha Univ.), Nakamura, H., Nishiura, M., Ito, M.A., Ashikawa, N.

Study on dust formation in plasma has been already started. Sizes and cross-sections of carbon dusts have been characterized by a scanning (SEM) and transmission (TEM) electron microscopes¹⁾. The SEM images indicate the productions of carbon dusts with an agglomeration of sub-micron size particles. Measured sizes of dusts are distributed for a wide range. Carbon dusts are considered to be generated from carbon re-deposition layers formed on a surface of a plasma-facing component. The time development of the agglomerations of carbon in a fusion device is one of most important information for fusion device development. However, the fundamental processes governing the dust growth have not been understood completely yet.

Information on the content of carbon in the edge plasma, as well as that on the form of carbon hydride molecules is indispensable to clarify the dust growth process in edge plasma. As one promising way to quantify is to measure the infrared absorption by hydrocarbon molecules, we propose to measure the infrared spectrum of the edge plasma to study carbon dust growth in the edge plasma.

In order to correlate the measured infrared absorption spectra of hydrocarbons and carbon clusters formation, an *ab initio* simulation code Gaussian $03^{2)}$ has been applied to calculate the vibration excitation levels of hydrocarbons and carbon clusters. Infrared absorption spectra for CH₄, C₂H₄, C₃H₄ have been calculated with the Gaussian 03 package under the density functional theory (DFT) in the present work. The results calculated with Gaussian 03 indicate that the infrared absorption spectroscopy is useful to investigate the time development of the agglomeration of carbon dusts in a fusion device.

Figure 1 shows an infrared absorption spectrum for CH_4 calculated with Gaussian 03. The major types of molecular vibrations consist of the stretching and bending vibrations in infrared wave number region. The bending vibration of C-H bond leads to lower wave number peak in Fig.1, and the stretching vibration of C-H bond results in the higher wave number peak. The lower and higher wave numbers multiplied by the above mentioned scaling factor are 1345.0 and 3044.7 cm⁻¹, respectively.

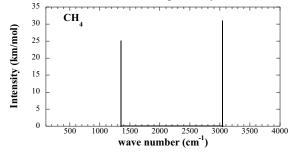


Fig.1 Infrared absorption spectra Calculated with Gaussian 03 for CH_4 .

Figures 2 shows the infrared absorption spectra for C_2H_2 calculated with the Gaussian 03. These calculated results indicate the number of peaks of infrared absorption spectra increase with increasing size of hydrocarbons. Namely, more absorption spectra appear as the structure of a hydrocarbon molecule becomes more complicated. These peaks consist of the bending and stretching vibrations for C-H bonds. The peaks of infrared absorption spectra for these carbon hydride molecules are expected to be measured in initial stage of carbon dust formation near the plasma facing wall in a fusion device. Thus, the time development of carbon hydride molecules leads to the change of infrared absorption spectra.

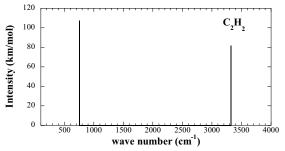


Fig.2 Infrared absorption spectra calculated with Gaussian 03 for C_2H_2 .

As the infrared absorption spectra depend on structures of molecules, the change in species composition of molecules in a fusion device should yield time dependent change in infrared absorption spectrum. Thus, agglomeration processes of carbon dusts can be characterized by monitoring infrared absorption spectra of the edge plasma during discharge operation.

A small experimental setup shown in Fig.3 to quantify the validity of infrared absorption spectroscopy through investigating the dust formation in a fusion device has been designed and is being built to see if dusts are actually formed from the apparatus without any starting carbon particle. The time development of the agglomeration of carbon dusts in the experimental setup is about to be observed by the infrared absorption spectroscopy. In addition to other low temperature plasma diagnostic tools like a Langmuir probe, infrared absorption spectra of carbon dust containing plasma will be constantly measured to study characteristic behaviour of plasma that forms carbon dusts.

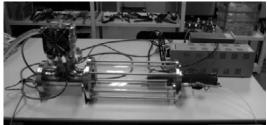


Fig. 3. Experimental setup.

- N. Ohno, M. Yoshimi, M. Tokitani, S. Takamura, K. Tokunaga, N. Yoshida : J. Nucl. Mater. **390-391** (2009) 61.
- 2) M. J. Frisch et al.: Gaussian, Inc., Wallingford CT, 2004.